propan-2-yl naphthalen-1-ylacetate

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 319 °C

Global applicability domain: Inside

Local applicability domain index: 5.74e-01

Confidence level: 8.09e-01

Nearest Neighbors from the Training Set

3-Ethoxy-1,1'-biphenyl
Measured: 305
Predicted: 294

2,2'-Dimethoxybiphenyl
Measured: 308
Predicted: 314

3,3'-Dimethoxy-1,1'-biphenyl
Measured: 328
Predicted: 314

Benzene, 1,1'-ethylidenebis(4-chloro-
Measured: 320
Predicted: 321